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Signal denoising and active learning for multiplexing spectrometer

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Inelastic neutron scattering instruments allow detailed studies of the dynamical structure factor, $S(Q,\omega)$, where Q is a scattering vector in reciprocal space and $h\omega = \Delta E$ an energy transfer. One of the work horses of modern neutron scattering is the triple-axis instrument, which typically have a high neutron flux and good energy resolution.Novel multiplexing triple-axis neutron scattering spectrometers yield significant improvements to the common triple-axis concept. Standard triple-axis (TAS) instruments cover only a single $(Q, h\omega)$-position per acquisition time, which leads to isolated trajectories mapped along lines of ω or Q during experiments. Multiplexing triple-axis instruments extend the triple-axis concept by employing multiple analysers and detectors. This allows for simultaneous measurements of large $S(Q,\omega)$ regions (increased data acquisition rate), while preserving a high neutron flux. Thanks to the recent development of the software package MJOLNIR, we are now able to manipulate and visualize data of the multiplexing spectrometer CAMEA at Paul Scherrer Insitute.

This boost in the data collection rate necessitates a rapid analysis of the scattered neutrons. However, current analysis strategies require experts to manually go through each dataset and mask out spurious background features. Being a notoriously slow process, conventional analysis methods are further based on defining narrow selections around a presumed signal while the rest of the dataset is discarded. In this work, we introduce a regularized model that enables to capture the background noise by separating it from the signal. The key idea is to exploit the rotation invariance property of the background and the sparsity of the signal to enforce a suited decomposition $Y = X + B$, where Y is the (noisy) observation dataset, X is the captured signal and B the captured background.

Another issue raised with the use of CAMEA is the beam time that must be budgeted carefully among contending experiments. Thus, it is crucial to ensure the optimal use of the time allocated to each experiment through an automated intelligent decision making system that will determine when sufficient data has been collected in an arbitrary measurement setting. To address this issue, we model the dispersion signal as a Gaussian Process that provides uncertainty estimation. Leveraging this confidence level, we can determine a data collection stopping time with respect to a given acceptance threshold. This will help CAMEA users to avoid beamlight overuse when a sufficient amount of data has been collected. We believe that the presented machine learning tools can be adapted to the use of different scattering instrument.

Primary authors: COHEN, Victor (Swiss Data Science Center (SDSC) - ETH Zurich); Dr LASS, Jakob (Paul Scherrer Institut); Dr BÉJAR HARO, Benjamin (Swiss Data Science Center (SDSC) - Paul Scherrer Institut); Dr MAZZONE, Daniel (Paul Scherrer Institut)

Presenter: Dr MAZZONE, Daniel (Paul Scherrer Institut)

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